FINAL TECHNICAL REPORT

Period: 1 February 1992 – 31 January 1993

Title of proposal: Calculation of molecular excitation rates

Award number: NCC 5–46

Institution: The Trustees of Columbia University in the City of New York

Principal investigator:

George Flynn
Professor of Chemistry
Columbia University
(212) 854–4162

State–to–state collisional excitation rates for interstellar molecules observed by radioastronomers continue to be required to interpret observed line intensities in terms of local temperatures and densities. A problem of particular interest is collisional excitation of water which is important for modeling the observed interstellar masers. In earlier work supported by a different NASA Grant, we studied excitation of water in collisions with He atoms; after many years of successively more refined calculations that problem now seems to be well understood, and discrepancies with earlier experimental data for related (pressure broadening) phenomena are believed to reflect experimental errors.

Because of interstellar abundances, excitation by H_2, the dominant interstellar species, is much more important than excitation by He, although it has been argued that rates for excitation by these are similar. Under the current grant we have begun theoretical study of this problem which is greatly complicated by the additional degrees of freedom which must be included both in determining the interaction potential and also in the molecular scattering calculation.

We have now computed the interaction forces for nearly a thousand molecular geometries and are close to having an acceptable global fit to these points which is necessary for the molecular dynamics calculations. Also, extensive modifications have been made to the molecular scattering code, MOLSCAT. These included coding the rotational basis sets and coupling matrix elements required for collisions of an asymmetric top with a linear rotor. We also incorporated a new method for numerical solution of the coupled equations. Because of the long–ranged nature of the water–hydrogen interaction it is necessary to integrate the equations to rather large intermolecular separations, and the integration methods previously available in MOLSCAT are not ideal for such cases. However, the method used by Alexander in his HIBRIDON code is particularly suited for such cases. We have obtained this code and incorporated that part which solves the coupled differential equations as an

option in the MOLSCAT program.

This work is being continued by Dr. Timothy Phillips, the post–doctoral student supported by this award, who is now a contract employee at NASA/Goddard Space Flight Center, Institute for Space Studies under the direction of Dr. Sheldon Green.

No inventions have been made in the performance of research covered by this grant.

Publications resulting from research under NASA Award NCC 5–46

1. S. Green, "Collisional excitation of formaldehyde in 'hot' interstellar molecular regions", Astrophys. J. (Suppl.) 76, 979–983 (1991).
2. S. Maluendes, A.D. McLean, and S. Green, "Comment on broadening of water microwave lines by collisions with He atoms", J. Chem. Phys. **96**, 8150–8156 (1992).
3. B.E. Turner, K.–W. Chan, S. Green, and D.A. Lubowich, "Tests of shock chemistry in IC 443 G", Astrophys. J. **399**, 114–133 (1992).
4. S. Green, S. Maluendes, and A.D. McLean, "Improved collisional excitation rates for interstellar water", Astrophys. J. Suppl. **85**, 181–185 (1993).